

Hexadecyl formate

Inchi:	InChI=1S/C17H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-17-18/h17H,2-16H2,1
InchiKey:	NZHKUCFYLBRISS-UHFFFAOYSA-N
Formula:	C17H34O2
SMILES:	CCCCCCCCCCCCCCCCOC=O
Mol. weight [g/mol]:	270.45
CAS:	4113-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-112.26	kJ/mol	Joback Method
hf	-612.01	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.641		Crippen Method
mvol	257.830	ml/mol	McGowan Method
pc	1281.91	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	659.44	K	Joback Method
tc	824.45	K	Joback Method
tf	345.58	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.34	J/molxK	659.44	Joback Method
cpg	814.38	J/molxK	796.95	Joback Method
cpg	799.24	J/molxK	769.45	Joback Method
cpg	783.38	J/molxK	741.95	Joback Method
cpg	766.79	J/molxK	714.44	Joback Method
cpg	749.45	J/molxK	686.94	Joback Method
cpg	828.83	J/molxK	824.45	Joback Method

dvisc	0.0001198	Paxs	659.44	Joback Method
dvisc	0.0001603	Paxs	607.13	Joback Method
dvisc	0.0002264	Paxs	554.82	Joback Method
dvisc	0.0003438	Paxs	502.51	Joback Method
dvisc	0.0005753	Paxs	450.20	Joback Method
dvisc	0.0011019	Paxs	397.89	Joback Method
dvisc	0.0025699	Paxs	345.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.31402e+01
Coeff. B	-8.61965e+03
Coeff. C	-1.21336e+02
Temperature range (K), min.	498.52
Temperature range (K), max.	604.81

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R543187&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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